1,3-Dimethyl-2,4,6-tris(chloromethyl)benzene

Inchi: InChI=1S/C11H13Cl3/c1-7-9(4-12)3-10(5-13)8(2)11(7)6-14/h3H,4-6H2,1-2H3
InchiKey: ZWXFQYBSJMBRNK-UHFFFAOYSA-N
Formula: C11H13Cl3
SMILES: Cc1c(CCl)cc(CCl)c(C)c1CCl
Mol. weight [g/mol]: 251.58

Physical Properties

Property code	Value	Unit	Source
gf	79.84	kJ/mol	Joback Method
hf	-126.94	kJ/mol	Joback Method
hfus	29.32	kJ/mol	Joback Method
hvap	58.16	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	4.520		Crippen Method
mcvol	178.810	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
rinpol	1953.00		NIST Webbook
tb	609.97	K	Joback Method
tc	830.14	K	Joback Method
tf	379.99	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.84	J/mol×K	609.97	Joback Method
cpg	394.21	J/mol×K	646.66	Joback Method
cpg	405.89	J/mol×K	683.36	Joback Method
cpg	416.89	J/mol×K	720.05	Joback Method
cpg	427.24	J/mol×K	756.75	Joback Method
cpg	436.97	J/mol×K	793.44	Joback Method
cpg	446.08	J/mol×K	830.14	Joback Method
dvisc	0.0010599	Pa×s	379.99	Joback Method
dvisc	0.0007054	Pa×s	418.32	Joback Method

dvisc	0.0005027	Pa×s	456.65	Joback Method
dvisc	0.0003775	Pa×s	494.98	Joback Method
dvisc	0.0002954	Pa×s	533.31	Joback Method
dvisc	0.0002389	Pa×s	571.64	Joback Method
dvisc	0.0001984	Pa×s	609.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R520302&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume